Triplet-Phase Measurements in Crystallography - an Application of Triple Correlation Theory from Speckle Imaging

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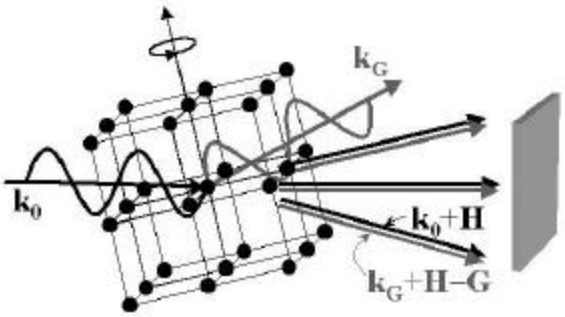

We present a recent advance towards solving the phase problem in x-ray crystallography using a *reference-beam diffraction* (RBD) technique [1,2]. This technique incorporates the principle of three-beam interference into the popular oscillating-crystal method in crystallography and allows parallel recordings of many three-beam interference profiles on an area detector. From these measured interference profiles a large number of triplet-phases of the reflections involved can be obtained. These measured phases can then be used in conjunction with the direct methods to solve a crystal structure, without the need for heavy atoms.

The RBD phasing technique in fact can be viewed as a direct application of the triple correlation or bispectrum processing method in speckle imaging [3,4]. A recursive phase retrieval scheme can thus be applied on the triplet-phases measured in a single RBD data set to obtain potentially all individual structure-factor phases of a given structure. This is being investigated as an alternative strategy to solve the phase problem in x-ray crystallography.

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1. Q. Shen, *Phys. Rev. Lett.* 80, 3268 (1998); *Phys. Rev.* B59, 11109 (1999).
2. Q. Shen, S. Kycia, and I. Dobrianov, *Acta Cryst.* A56, 268 (2000).
3. A.W. Lohmann, G. Weigeit, and B. Wirnitzer, *Appl. Opt.* 22, 4028 (1983).
4. R.P. Millane, *J. Opt. Soc. Am.* A7, 394 (1990).